

10678836

=> d his

(FILE 'HOME' ENTERED AT 11:52:46 ON 28 JAN 2005)

FILE 'REGISTRY' ENTERED AT 11:53:02 ON 28 JAN 2005

L1 STRUCTURE UPLOADED  
L2 0 S L1  
L3 15 S L1 SSS FULL

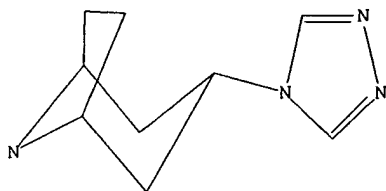
FILE 'CAPLUS' ENTERED AT 11:53:31 ON 28 JAN 2005

L4 4 S L3

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> d 1-4 bib abs hitstr.

L4 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:996153 CAPLUS

DN 141:424115

TI Preparation of N-phenylalkyl piperidines and 8-azabicyclo[3.2.1]octanes as CCR5 receptor modulators

IN Cumming, John; Faull, Alan

PA Astrazeneca AB, Swed.

SO PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004099178	A1	20041118	WO 2004-SE697	20040506
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW:				
	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI SE 2003-1369 A 20030509

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [wherein A = absent, CH<sub>2</sub>CH<sub>2</sub>; R<sub>1</sub> = halo, OH, NO<sub>2</sub>, CN, alkyl, alkoxy, (CH<sub>2</sub>)<sub>n</sub>SO<sub>2</sub>-2-alkyl, (un)substituted (CH<sub>2</sub>)<sub>n</sub>SO<sub>2</sub>NH<sub>2</sub>, NH<sub>2</sub>, CONH<sub>2</sub>, Ph, heteroaryl, ureido, etc.; R<sub>2</sub> = (halo)phenyl; (halo)thienyl; R<sub>3</sub> = H, Me; R<sub>4</sub> = (un)substituted heterocyclyl; n = 0-2; and pharmaceutically acceptable salts or solvates thereof] were prepared as chemokine CCR5 receptor modulators. For example, (R)-3-(3-fluorophenyl)-3-(4-methanesulfonylphenyl)propionaldehyde was coupled with 5-methanesulfonyl-1-(piperidin-4-yl)-1H-benzimidazole in the presence of sodium trisacetoxyborohydride and AcOH in CH<sub>2</sub>Cl<sub>2</sub> to give II. The latter inhibited binding of MIP-1 $\alpha$  to recombinant human CCR5 receptors

expressed in membranes prepared from Chinese hamster ovary cells with a  $\text{Pic}_{50}$  (i.e., the neg. log of the  $\text{IC}_{50}$  value) of 9.0. Thus, I and pharmaceutical comps. comprising them are useful for treating a CCR5 mediated diseases, such as autoimmune and inflammatory disorders (no data).

**IT 795311-21-6P**

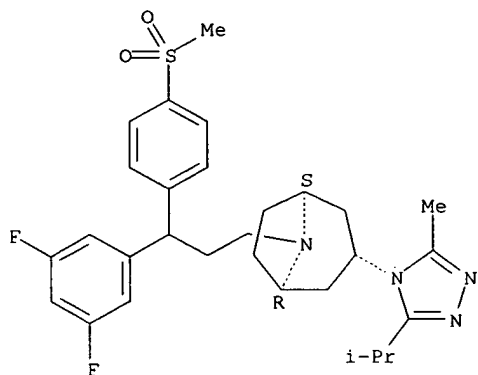
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(CCR5 modulator; preparation of N-phenylalkyl piperidines and azabicyclo[3.2.1]octanes as CCR5 receptor modulators for treatment of autoimmune and inflammatory disorders)

RN 795311-21-6 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[3-(3,5-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]propyl]-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-, (3-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



**IT 423165-07-5P 423165-13-3P**

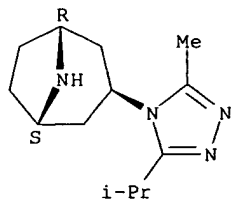
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of N-phenylalkyl piperidines and azabicyclo[3.2.1]octanes as CCR5 receptor modulators for treatment of autoimmune and inflammatory disorders)

RN 423165-07-5 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-, (3-exo)- (9CI) (CA INDEX NAME)

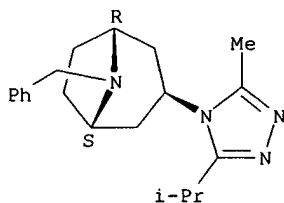
Relative stereochemistry.



RN 423165-13-3 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-(phenylmethyl)-, (3-exo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN  
AN 2004:534173 CAPLUS  
DN 141:89016  
TI Preparation of benzimidazolylazabicyclooctylethylpiperidines as Ccr5  
antagonists for the treatment of HIV infection  
IN Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph; Bifulco, Neil;  
Boros, Eric Eugene; Chauder, Brian Andrew; Chong, Pek Yoke; Duan,  
Maosheng; Deanda, Felix, Jr.; Koble, Cecilia Suarez; Mclean, Ed Williams;  
Peckham, Jennifer Poole; Perkins, Angilique C.; Thompson, James Benjamin;  
Vanderwall, Dana  
PA Smithkline Beecham Corporation, USA; et al.  
SO PCT Int. Appl., 859 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004054974	A2	20040701	WO 2003-US39644	20031212
WO 2004054974	A3	20040902		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI US 2002-433634P	P	20021213		
OS MARPAT 141:89016				
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Compds. I [R1 = (optionally substituted) alkyl, aryl, heteroaryl, carbocyclyl; R2 = H, (optionally substituted) alkyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, aralkyl, heteroarylalkyl, heteroarylcycloalkyl, aralkylcarbonyl, heteroarylsulfinyl; R3 = H, halo, cyano, trifluoromethyl, (optionally substituted) amino, acylamino, alkyl; X = C1-5 alkylene, optionally substituted with oxo or thioxo groups or halogen atoms, and optionally containing 1-3 oxygen, nitrogen, sulfur, or phosphorus atoms; Y = carbonyl, thiocarbonyl, 1,2-dioxoethylene, oxyalkylcarbonyl, sulfinyl, sulfonyl, oxycyanoimino, (optionally substituted) aminocarbonyl, carbonylamino, aminothiocabonyl, oxyiminomethyl, thioiminomethyl, amino(cyanoimino)methyl, (cyanoimino)methyl, amino(acylimino)methyl, amino(sulfonylimino)methyl, amino(sulfinylimino)methyl, amino(alkoxyimino)methyl, amino(imino)methyl, (cyanoimino)methoxy, iminomethoxy, (cyanoimino)methanethiyl, alkylcarbonyloxy; A = saturated, partially saturated, or aromatic monocyclic ring with 5-6 atoms or a bicyclic ring with 8-10 members containing 0-5 nitrogen, oxygen, and/or sulfur atoms] such as II are prepared I are prepared as Ccr5 antagonists for the treatment of viral infections, (particularly HIV infection), related syndromes such as AIDS-related complex (ARC), progressive generalized lymphadenopathy, Kaposi's sarcoma, and neurol. conditions, and other diseases such as multiple sclerosis, rheumatoid arthritis, Crohn's disease, and immune-mediated disorders. The invention

comps. have pIC50 values of  $\geq 5$  in assays for Ccr5 antagonism. Piperidineacetaldehyde III is prepared in four steps from 4-phenyl-4-piperidinecarbonitrile by protection of the piperidine with Boc anhydride, reduction of the nitrile with diisobutylaluminum hydride, Wittig olefination with methoxymethylphosphonium chloride, and hydrolysis of the enol ether with catalytic p-toluenesulfonic acid monohydrate. The hydrochloride of endo-(benzimidazolyl)azabicyclooctane IV is prepared in five steps from tert-Bu endo-3-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate; reductive amination with benzylamine, reductive cleavage of the benzyl group by palladium-mediated hydrogenation, a nucleophilic aryl substitution reaction with 1-fluoro-2-nitrobenzene, reduction of the nitro group by hydrogenation over palladium on carbon, and treatment with tri-Et orthoacetate followed by treatment with hydrochloric acid in ethanol. Coupling of III and IV by reductive amination with sodium triacetoxyborohydride, cleavage of the Boc group with hydrochloric acid in dioxane, and acylation with pivaloyl chloride and triethylamine yields II.

IT **716351-59-6P**

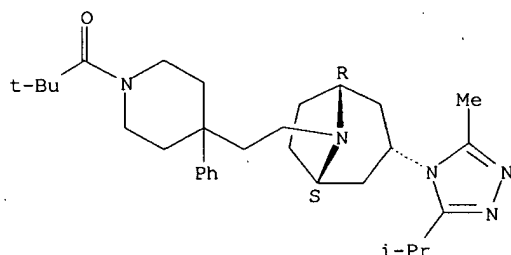
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzimidazolylazabicyclooctylethylpiperidine Ccr5 antagonists in the treatment of bacterial and viral infections and other diseases)

RN 716351-59-6 CAPLUS

CN Piperidine, 1-(2,2-dimethyl-1-oxopropyl)-4-[2-[(3-endo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]ethyl]-4-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:951304 CAPLUS

DN 140:193031

TI Method for identification of a ligand whereby receptor residence time is measured

IN Dorr, Patrick Karl; Perros, Manoussos; Rickett, Graham Anthony

PA Pfizer Limited, UK; Pfizer Inc.

SO PCT Int. Appl., 51 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003100427	A1	20031204	WO 2003-IB2023	20030514
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2004023845	A1	20040205	US 2003-442358	20030520
PRAI	GB 2002-11923	A	20020523		
	GB 2003-9392	A	20030424		
	US 2002-386996P	P	20020607		
AB	The invention relates to the use of an assay that measures receptor residence time of a ligand on its receptor in vitro for the identification				

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of a ligand for that receptor predicted to be efficacious in vivo in the treatment of a disease that responds to modulation of that receptor's natural function.

IT 376348-65-1

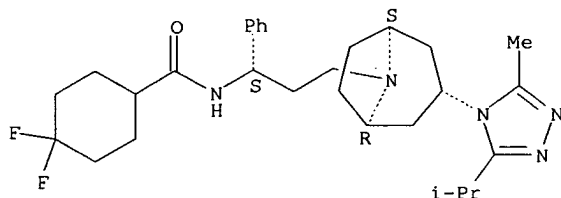
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(method for identification of ligand whereby receptor residence time is measured)

RN 376348-65-1 CAPLUS

CN Cyclohexanecarboxamide, 4,4-difluoro-N-[(1S)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2001:868452 CAPLUS

DN 136:6195

TI Preparation of therapeutic tropane derivatives

IN Perros, Manoussos; Price, David Anthony; Stammen, Blanda Luzia Christa; Wood, Anthony

PA Pfizer Limited, UK; Pfizer Inc.

SO PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DT Patent

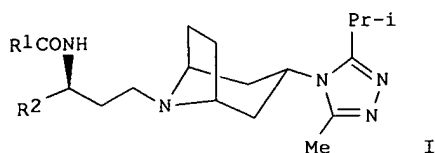
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001090106	A2	20011129	WO 2001-IB806	20010509
	WO 2001090106	A3	20020328		
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	CA 2408909	AA	20011129	CA 2001-2408909	20010509
	EP 1284974	A2	20030226	EP 2001-925808	20010509
	EP 1284974	B1	20040303		
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	BR 2001010955	A	20030603	BR 2001-10955	20010509
	JP 2003534343	T2	20031118	JP 2001-586293	20010509
	AT 260914	E	20040315	AT 2001-925808	20010509
	EE 200200656	A	20040615	EE 2002-656	20010509
	PT 1284974	T	20040630	PT 2001-925808	20010509
	NZ 521477	A	20040730	NZ 2001-521477	20010509
	ES 2215129	T3	20041001	ES 2001-1925808	20010509
	US 2002013337	A1	20020131	US 2001-865950	20010525
	US 6667314	B2	20031223		
	BG 107140	A	20030530	BG 2002-107140	20020923
	NO 2002005227	A	20021031	NO 2002-5227	20021031
	ZA 2002009516	A	20031022	ZA 2002-9516	20021122
	US 2004067977	A1	20040408	US 2003-678836	20031003
PRAI	GB 2000-14046	A	20000526		
	GB 2000-15835	A	20000627		
	US 2000-214587P	P	20000627		

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US 2000-219202P P 20000719  
 WO 2001-IB806 W 20010509  
 US 2001-865950 A1 20010525  
 OS MARPAT 136:6195  
 GI



AB The tropanes I (R1 = C3-6 cycloalkyl optionally substituted by one or more fluorine atoms, C1-6 alkyl optionally substituted by one or more fluorine atoms, C3-6 cycloalkylmethyl optionally ring-substituted by one or more fluorine atoms; R2 = Ph optionally substituted by one or more fluorine atoms) and their pharmaceutically acceptable salts and solvates were prepared. Thus, (1S)-3-[(3-isopropyl-5-methyl-4H-1,2,4-triazol-4-yl)-exo-8-azabicyclo[3.2.1]oct-8-yl]-1-phenyl-1-propanamine, preparation given, was treated with cyclobutanecarboxylic acid in presence of polymer bound N-benzyl-N'-cyclohexylcarbodiimide to give I (R1 = cyclobutyl, R2 = Ph). I had an IC50 value of less than 10nM in the assay for CCR5 binding.

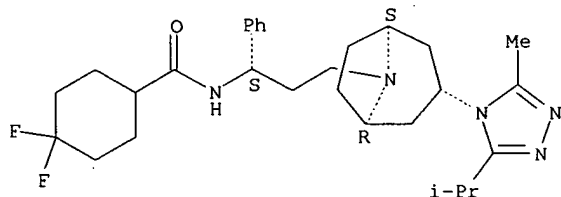
IT **376348-65-1P**

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of tropane derivs. as CCR5 receptor antagonists)

RN 376348-65-1 CAPLUS

CN Cyclohexanecarboxamide, 4,4-difluoro-N-[(1S)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **376348-62-8P 376348-63-9P 376348-64-0P**

**376348-66-2P**

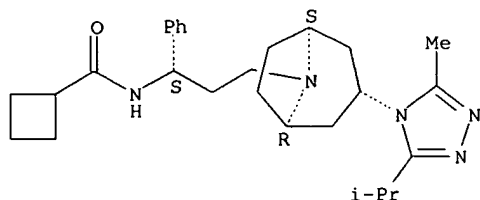
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of tropane derivs. as CCR5 receptor antagonists)

RN 376348-62-8 CAPLUS

CN Cyclobutanecarboxamide, N-[(1S)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

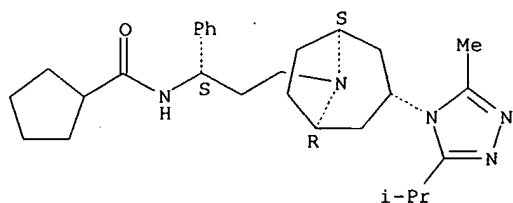


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RN 376348-63-9 CAPLUS

CN Cyclopentanecarboxamide, N-[(1S)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl]- (9CI) (CA INDEX NAME)

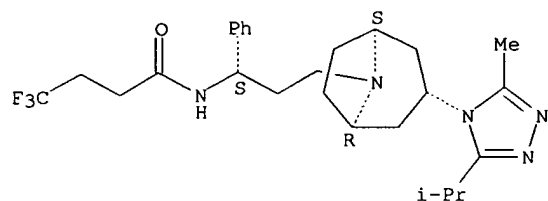
Absolute stereochemistry. Rotation (-).



RN 376348-64-0 CAPLUS

CN Butanamide, 4,4,4-trifluoro-N-[(1S)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl]- (9CI) (CA INDEX NAME)

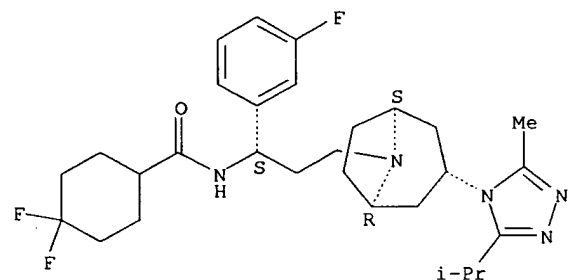
Absolute stereochemistry. Rotation (-).



RN 376348-66-2 CAPLUS

CN Cyclohexanecarboxamide, 4,4-difluoro-N-[(1S)-1-(3-fluorophenyl)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 376348-71-9

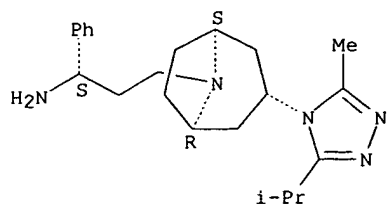
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of tropane derivs. as CCR5 receptor antagonists)

RN 376348-71-9 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanamine, 3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]- $\alpha$ -phenyl-, ( $\alpha$ S,3-exo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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IT 376348-70-8P 376348-72-0P 376348-73-1P

376348-80-0P

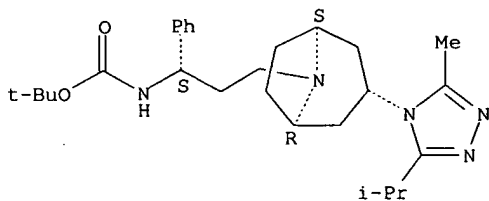
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tropane derivs. as CCR5 receptor antagonists)

RN 376348-70-8 CAPLUS

CN Carbamic acid, [(1S)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

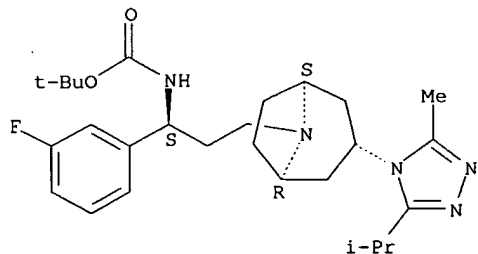
Absolute stereochemistry.



RN 376348-72-0 CAPLUS

CN Carbamic acid, [(1S)-1-(3-fluorophenyl)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

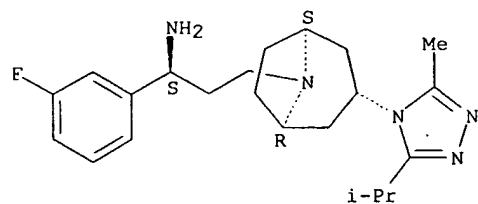
Absolute stereochemistry.



RN 376348-73-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanamine,  $\alpha$ -(3-fluorophenyl)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-, ( $\alpha$ S,3-exo)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





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RN 376348-80-0 CAPLUS

CN Carbamic acid, [(1S)-3-[(3-exo)-3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-azabicyclo[3.2.1]oct-8-yl]-1-phenylpropyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

